HEAT TRANSPORT IN A THREE DIMENSIONAL SLAB GEOMETRY AND THE TEMPERATURE PROFILE OF INGEN-HAUSZ'S EXPERIMENT

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We study the transport of heat in a three dimensional, harmonic crystal of slab geometry whose boundaries and the intermediate surfaces are connected to stochastic, white noise heat baths at different temperatures. Heat baths at the intermediate surfaces are required to fix the initial state of the slab in respect of its surroundings. We allow the energy fluxes flown between the intermediate surfaces and the attached baths and impose conditions that relate the widths of Gaussian noises of the intermediate baths. We show that under those conditions Fourier's law holds in the continuum limit. We obtain an exponentially falling temperature profile from high to low temperature end of the slab and this nature was already confirmed by Ingen-Hausz's experiment. Profile indicates that transport in the steady state involves the processes of conduction and radiation of heat.

Keywords: Heat conduction; Langevin equation

1. Introduction

We take a piece of solid bar and establish a steady temperature gradient between its two ends. The rest part of the bar remains exposed to the environment. The transport of heat involves three processes such as, conduction, radiation and absorption of heat. In the steady state absorption is absent and the conducted current density $\mathbf{J}(\mathbf{x})$ obeys Fourier's law:

$$\mathbf{J}(\mathbf{x}) = -\kappa \nabla T(\mathbf{x}), \tag{1}$$

where $\nabla T(\mathbf{x})$ be the local temperature gradient and κ is known as the thermal conductivity of the solid. In the steady state the temperature profile of the bar

is exponentially falling from high to low temperature end and this very nature was already confirmed by the experiment performed by Ingen-Hausz[14]. Since the transport of heat is a non-equilibrium process, it becomes a theoretical challenge to derive Fourier's law and the exponentially falling temperature profile from the application of non-equilibrium statistical mechanics to a basic model of solid. It is observed that the heat transport in one dimension exhibits anomalous[2] behaviour. It means that the thermal conductivity shows a power law dependence $\kappa \sim N^{\alpha}$, where N be the linear size of the system. There are models which predict divergent ($0 < \alpha < 1$) thermal conductivity [1,2,3,4,5,6] in one dimension. Numerical study indicates a logarithmic divergence[7] of thermal conductivity $\kappa \sim \ln N$ in two dimension. A power law behaviour[8] is also observed in such a system. The validity of Fourier's law is confirmed numerically[9] in one and two dimensional systems with pining and anharmonicity. It has been shown numerically[10] that a normal transport takes place in the disordered harmonic crystal in three dimension, subjected to an external pining potential. The validity of this law is also established using a simulation study[11] in three dimensional anharmonic crystal. This study provides a temperature profile which is almost linear and very little concave in the upward direction.

It is worthy to be mentioned of an interesting model of harmonic crystal with 'self-consistent' stochastic heat baths[12]. A rigorous derivation shows that the Fourier's law holds in dimension one of this model. However, for a d dimensional crystal, when d is very large, the heat conductivity is shown to behave as $(l_d d)^{-1}$, where l_d is the coupling to the intermediate reservoirs. Using 'self-consistent' heat baths one fixes the flow of energy fluxes between the intermediate sites and the attached baths to zero and these conditions give rise to a temperature profile which falls linearly from high to low temperature end of the slab. In this paper we use the same model in three dimension only, without the on-site binding potential in the Hamiltonian. Instead of using 'self-consistent' baths, we allow the heat fluxes to be flown between the intermediate surfaces and the attached baths and impose conditions among the Gaussian widths of the noises of intermediate heat baths. We show that under these conditions Fourier's law holds in the continuum limit and the temperature profile exhibits an exponential fall from high to low temperature end of the slab. A similar profile was obtained experimentally long before by Ingen Hausz. In general, the temperature profile provides an idea about the underlying physical processes[14] that may take place owing to transport of heat in the steady state limit. The transport in our model involves the conduction and radiation of heat. On the other hand using 'self-consistent' heat baths[12], one disregards radiation from the transport process of heat.

We organize the paper in the following manner. We introduce the model and give the steady state solution of the Langevin's equation in Section 2. We evaluate different correlators involving normal coordinates and normal velocities in Section 3. We give the derivation of the exact temperature profile of the slab and discuss its experimental consequences in Section 4. This section also contains the derivation of Fourier's law in the continuum limit. The discussion of our results and the conclusion

are given in Section 5.

2. Model

We consider a cubic crystal in three dimension. The form of the Hamiltonian

$$H = \sum_{\mathbf{n}} \frac{\dot{x}_{\mathbf{n}}^2}{2} + \sum_{\mathbf{n},\hat{\mathbf{e}}} \frac{1}{2}(x_{\mathbf{n}} - x_{\mathbf{n}+\hat{\mathbf{e}}})^2. \tag{2}$$

The displacement field $x_{\mathbf{n}}$ is defined on each lattice site $\mathbf{n} = (n_1, n_2, n_3)$ where $n_1 = 1, \cdots, N$, $n_2 = 1, \cdots, W_2$, and $n_3 = 1, \cdots, W_3$. Here $\hat{\mathbf{e}}$ denotes the unit vector in the three directions. We choose the value of mass attached to each lattice point and the harmonic spring constant as one. We have Langevin's type heat baths that are coupled to the surfaces at $n_1 = 1$ and $n_1 = N$ and are maintained at fixed temperatures T_1 and T_N ($T_1 > T_N$) respectively. Apart from these two heat baths, the surroundings play a key role to fix the initial state of the slab. Suppose, the heat baths are removed from the two end surfaces of the slab. In this situation we expect that the temperature of the slab must be equal to the temperature of the surroundings in the stationary state limit. To achieve this expectation, in addition to two heat baths that are already fixed at the end surfaces of the slab, we require to couple $N-2$ more Langevin's type heat baths at the intermediate surfaces from $n_1 = 2$ to $n_1 = N-1$. To deal with the same problem in one dimension an equilibrium phase space distribution has been assumed to fix the initial state of the system[1]. Now the equation of motion of a particle at the site $\mathbf{n}$ reads

$$\ddot{x}_{\mathbf{n}} = -\sum_{\hat{\mathbf{e}}}(x_{\mathbf{n}} - x_{\mathbf{n}+\hat{\mathbf{e}}}) - \gamma \dot{x}_{\mathbf{n}} + \eta_{\mathbf{n}}. \tag{3}$$

We have chosen the noises to be white and they are uncorrelated at different sites. Assuming the process to be Gaussian, the noise correlation is specified by

$$\langle \eta_{\mathbf{n}}(t) \eta_{\mathbf{n}'}(t') \rangle = \gamma z_{n_1} \delta(t-t') \delta_{\mathbf{n},\mathbf{n}'}. \tag{4}$$

According to ref. [12], z_{n_1} is chosen to be proportional to the temperature of the corresponding layer. However, we determine them in our model using fluctuation dissipation theorem. We use the following periodic boundary conditions for the displacement field and the noise:

$$\begin{aligned} x_{\mathbf{n}+(0,W_2,0)}(t) &= x_{\mathbf{n}}(t) = x_{\mathbf{n}+(0,0,W_3)}(t) \\ \eta_{\mathbf{n}+(0,W_2,0)}(t) &= \eta_{\mathbf{n}}(t) = \eta_{\mathbf{n}+(0,0,W_3)}(t) \end{aligned} \tag{5}$$

These boundary conditions lead to the following expansion for $x_{\mathbf{n}}(t)$ and $\eta_{\mathbf{n}}(t)$:

$$x_{\mathbf{n}}(t) = \frac{1}{\sqrt{W_2 W_3}} \sum_{\mathbf{p}} y_{n_1}(\mathbf{p}, t) \mathrm{e}^{i\mathbf{p}.\mathbf{n}_\perp a}, \tag{6}$$

$$\eta_{\mathbf{n}}(t) = \frac{1}{\sqrt{W_2 W_3}} \sum_{\mathbf{p}} f_{n_1}(\mathbf{p}, t) \mathrm{e}^{i\mathbf{p}.\mathbf{n}_\perp a}, \tag{7}$$

where a be the lattice constant of the crystal, $\mathbf{p} = (p_2, p_3)$ and $\mathbf{n}_\perp = (n_2, n_3)$. Upon substitution of eq. (6) and (7) into eq. (3) we obtain

$$\ddot{y}_j = -\sum_{k=1}^{N} V_{jk} y_k - \gamma \dot{y}_j + f_j \tag{8}$$

where the $N \times N$ matrix

$$V = \begin{pmatrix} 2\omega_0^2 & -1 & 0 & 0 & \dots \\ -1 & 2\omega_0^2 & -1 & 0 & \dots \\ 0 & -1 & 2\omega_0^2 & -1 & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \\ 0 & \dots & 0 & -1 & 2\omega_0^2 \end{pmatrix} \tag{9}$$

and

$$\omega_0^2(\mathbf{p}) = 1 + 2\sin^2(\frac{p_2 a}{2}) + 2\sin^2(\frac{p_3 a}{2}). \tag{10}$$

We have assumed here that $y_0(\mathbf{p}, t) = 0 = y_{N+1}(\mathbf{p}, t)$. To solve eq. (8) we diagonalize the matrix V. The solution of the N order polynomial equation $\left|V - \alpha^2 I\right| = 0$ gives the eigenvalues of V as

$$\alpha_k^2(\mathbf{p}) = 2\omega_0^2(\mathbf{p}) + 2\cos\left(\frac{k\pi}{N+1}\right). \tag{11}$$

The j-th component of the normalized eigenvector corresponding to the eigenvalue α_k^2 is given by

$$a_j^{(k)} = \sqrt{\frac{2}{N+1}}(-1)^{j+1}\sin\left(\frac{jk\pi}{N+1}\right). \tag{12}$$

The diagonalizing matrix A thus reads as $A_{jk} = a_j^{(k)}$ such that $A^T A = I$ and $A^T V A = \alpha^2$, where $(\alpha^2)_{jk} = \alpha_j^2\, \delta_{jk}$. We introduce a new set of coordinates ξ_j as

$$y_j(\mathbf{p}, t) = \sum_{k=1}^{N} A_{jk} \xi_k(\mathbf{p}, t). \tag{13}$$

The equation of motion of ξ_j in matrix form can be written as

$$\ddot{\xi} = -\alpha^2 \xi - \gamma \dot{\xi} + \tilde{f}, \tag{14}$$

where $\tilde{f} = A^T f$. Since the matrix V is diagonal with respect to ξ_j $(j = 1, \cdots, N)$, we henceforth refer them as normal coordinates. It is evident from this equation that each normal mode is acted on by dissipative force and noise offered by the heat baths. Moreover, one normal mode is coupled to the other through noise terms. The couplings among normal coordinates lead to the flow of energy from one mode to the other and thereby leading to a non-ballistic flow of heat in the slab. In the

steady state limit ($t >> 1/\gamma$) we are interested in the particular solution of the equations of motion of ξ. We use the Fourier transform of

$$\xi_j(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \xi_j(\omega) \mathrm{e}^{i\omega t} \text{ and } f_j(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f_j(\omega) \mathrm{e}^{i\omega t} \tag{15}$$

in eq. (14) and obtain

$$\xi_j(\mathbf{p}, \omega) = -\frac{\tilde{f}_j(\mathbf{p}, \omega)}{\omega^2 - \alpha_j^2(\mathbf{p}) - i\gamma\omega}. \tag{16}$$

Now upon substitution of eq. (16) into (15) we obtain

$$\xi_j(\mathbf{p}, t) = -\sum_{k=1}^{N} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\mathrm{e}^{i\omega t}}{\omega^2 - \alpha_j^2(\mathbf{p}) - i\gamma\omega} a_k^{(j)} f_k(\mathbf{p}, \omega). \tag{17}$$

Now the use of eq. (7) and (15) in (4) gives the noise correlation in frequency and wave-vector space as

$$\langle f_j(\mathbf{p}, \omega) f_k(\mathbf{p'}, \omega') \rangle = 2\pi\gamma z_j \delta_{j,k} \delta(\omega + \omega') \delta_{\mathbf{p}+\mathbf{p'},0}. \tag{18}$$

3. Correlation functions

For the purpose of calculating physically observable quantities in this model, such as temperature profile and heat current density, we require to obtain the correlation functions involving normal coordinates and velocities. First we compute the correlation between normal coordinate and normal velocity using eq. (17) and (18). We perform a frequency integration using delta function in frequency space and obtain the correlation as

$$\langle \xi_{k_1}(\mathbf{p}, t) \dot{\xi}_{k_2}(\mathbf{p'}, t') \rangle = \gamma I_c(t - t') \delta_{\mathbf{p}+\mathbf{p'},0} \sum_{j=1}^{N} a_j^{(k_1)} a_j^{(k_2)} z_j \tag{19}$$

where

$$\begin{aligned} & I_c(t - t') \\ & = -i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\omega \mathrm{e}^{i\omega(t-t')}}{(\omega^2 - \alpha_{k_1}^2 - i\gamma\omega)(\omega^2 - \alpha_{k_2}^2 + i\gamma\omega)}. \end{aligned} \tag{20}$$

Performing the integration over ω we obtain

$$I_c(t - t') = \frac{\mathrm{e}^{-\gamma|t-t'|/2}}{4\,\Delta_d(\beta_1, \beta_2)} [I_c^{>}(t - t')\theta(t - t') + I_c^{<}(t - t')\theta(t' - t)], \tag{21}$$

where

$$\Delta_d(\beta_1,\beta_2) = (\cos\beta_1 - \cos\beta_2)^2 + \gamma^2(2\omega_0^2(\mathbf{p}) + \cos\beta_1 + \cos\beta_2), \tag{22}$$

$$I_c^>(t-t') = 2(\cos\beta_1 - \cos\beta_2)\cos(\omega_{k_1}|t-t'|) + \frac{\gamma}{\omega_{k_1}}\{(4\omega_0^2 + 3\cos\beta_1 + \cos\beta_2)\sin(\omega_{k_1}|t-t'|)\}, \tag{23}$$

$$I_c^<(t-t') = 2(\cos\beta_1 - \cos\beta_2)\cos(\omega_{k_2}|t-t'|) - \frac{\gamma}{\omega_{k_2}}\{(4\omega_0^2 + \cos\beta_1 + 3\cos\beta_2)\sin(\omega_{k_2}|t-t'|)\}, \tag{24}$$

$$\beta_{1,2} = \pi k_{1,2}/(N+1), \tag{25}$$

$$\omega_{k_{1,2}} = \sqrt{\alpha_{k_{1,2}}^2 - \gamma^2/4}. \tag{26}$$

It is clear that $I_c(t-t') \to 0$, when $|t-t'| \to \infty$. When $t = t'$

$$I_c(0) = \frac{\cos\beta_1 - \cos\beta_2}{2\,\Delta_d(\beta_1,\beta_2)}. \tag{27}$$

We compute the equal time velocity-velocity correlation using eq. (17) and (18) and after performing the algebraic manipulation obtain the correlation as

$$\langle \dot{\xi}_{k_1}(\mathbf{p},t)\dot{\xi}_{k_2}(-\mathbf{p},t)\rangle = \frac{\gamma^2}{N+1}\frac{2\omega_0^2 + \cos\beta_1 + \cos\beta_2}{\Delta_d(\beta_1,\beta_2)} \times \sum_{j=1}^{N} z_j \sin(j\beta_1)\sin(j\beta_2). \tag{28}$$

4. Temperature profile and Fourier's law

Consider a particle on the surface at n_1. The mean square velocity of the particle in the steady state limit reads

$$v_m^2(n_1) = \frac{1}{W_2W_3}\sum_{\mathbf{n}_\perp}\langle \dot{x}_{\mathbf{n}}^2\rangle = \frac{1}{W_2W_3}\sum_{\mathbf{p}}\sum_{k_1,k_2=1}^{N} a_{n_1}^{(k_1)}a_{n_1}^{(k_2)}\langle \dot{\xi}_{k_1}(\mathbf{p},t)\dot{\xi}_{k_2}(-\mathbf{p},t)\rangle, \tag{29}$$

where we have used eq. (6) and (13) in the last step. Then we substitute eq. (12) and (28) in the above equation and evaluate p_2 and p_3 sum in the continuum limit. According to this limit, when $a \to 0$ and $W_{2,3} \to \infty$, $a\,W_{2,3}$ remain fixed and the discrete sums over p_2 and p_3 are converted into integrals:

$$\sum_{\mathbf{p}} \to \frac{a^2W_2W_3}{(2\pi)^2}\int_{-\frac{\pi}{a}}^{-\frac{\pi}{a}}\int_{-\frac{\pi}{a}}^{-\frac{\pi}{a}} dp_2\, dp_3. \tag{30}$$

Evaluation of the integrals[13] over p_2 and p_3 gives

$$v_m^2(n_1) = 2\sum_{j=1}^{N} C_{n_1,j}z_j \tag{31}$$

where

$$C_{n_1,j} = \frac{1}{(N+1)^2} \sum_{k_1,k_2=1}^{N} \frac{\Lambda(\beta_1,\beta_2)}{\Delta(\beta_1,\beta_2)} \sin(n_1\beta_1)\sin(n_1\beta_2)\sin(j\beta_1) \times \sin(j\beta_2), \tag{32}$$

$$\Lambda(\beta_1,\beta_2) = \Delta(\beta_1,\beta_2) - \{(\cos\beta_1 - \cos\beta_2)^2 \times F(1/2,1/2,1;(4\gamma^2/\Delta(\beta_1,\beta_2))^2)\}, \tag{33}$$

$$\Delta(\beta_1,\beta_2) = (\cos\beta_1 - \cos\beta_2)^2 + \gamma^2\,(6+\cos\beta_1+\cos\beta_2). \tag{34}$$

The $N \times N$ matrix C has the following properties:

$$C_{j,k} = C_{k,j} \quad \text{and} \quad C_{j,k} = C_{N+1-j,N+1-k}. \tag{35}$$

To thermalize the layers it is required that the average kinetic energy of a particle on a layer in the steady state limit coincides with its energy at thermal equilibrium. This requirement gives the following N simultaneous equations of z_k:

$$\sum_{k=1}^{N} C_{j,k} z_k = \frac{1}{2} T_j, \tag{36}$$

where we have chosen the Boltzmann constant $k_B = 1$. T_j is the temperature of the j-th layer. According to this equation, if $C_{j,k} = C_{j,j}\delta_{j,k}$, then only z_j will be proportional to T_j[12]. This equation also indicates that the system in the steady state consists of N different, thermally equilibriated sub-systems which are characterized by the temperatures $T_1, \cdots, T_N$. In eq. (36), T_1 and T_N are given. Apart from these two T_j for $2 \le j \le N-1$ and z_j for $1 \le j \le N$ are remained unknown. We require to know additional conditions which will facilitate us to obtain the temperature profile of the slab and the z_js as a solution of these N equations.

Since $T_1 > T_N$, there will be a rectilinear flow of heat from the left boundary surface at $n_1 = 1$ to the right boundary surface at $n_1 = N$ of the slab. Heat current density $j_{\mathbf{n}}$ from the lattice site $\mathbf{n}$ to $\mathbf{n} + \hat{\mathbf{e}}_1$, where $\hat{\mathbf{e}}_1 = (1,0,0)$, is given by[2]

$$j_{\mathbf{n}} = \frac{1}{2}\langle (x_{\mathbf{n}+\hat{\mathbf{e}}_1} - x_{\mathbf{n}})(\dot{x}_{\mathbf{n}+\hat{\mathbf{e}}_1} + \dot{x}_{\mathbf{n}})\rangle \tag{37}$$

The average heat current density per bond[11]

$$J = \frac{1}{W_2 W_3 (N-1)} \sum_{n_1=1}^{N-1} \sum_{n_2=1}^{W_2} \sum_{n_3=1}^{W_3} j_{\mathbf{n}}. \tag{38}$$

We substitute eq. (6) and (13) in J and after performing the summations over n_2 and n_3 obtain the average heat current density per bond in the steady state limit as

$$J = \frac{1}{2W_2W_3(N-1)} \sum_{\mathbf{p}} \sum_{k_1,k_2=1}^{N} \sum_{n_1=1}^{N-1} (a_{n_1+1}^{(k_1)} - a_{n_1}^{(k_1)})(a_{n_1+1}^{(k_2)} + a_{n_1}^{(k_2)}) \times \langle \xi_{k_1}(\mathbf{p},t)\dot{\xi}_{k_2}(-\mathbf{p},t)\rangle. \tag{39}$$

We now use eq. (12) and evaluate the sum over n_1. The result is given in the following:

$$\sum_{n_1=1}^{N-1}(a_{n_1+1}^{(k_1)} - a_{n_1}^{(k_1)})(a_{n_1+1}^{(k_2)} + a_{n_1}^{(k_2)}) = \frac{2}{N+1}(1-(-1)^{k_1+k_2})\sin\beta_1\sin\beta_2 \times\Big[\frac{1}{\cos\beta_2-\cos\beta_1}-1\Big]. \quad (40)$$

We use this result and also the eq. (19) and (27) in eq. (39). Then we evaluate the discrete sums over p_2 and p_3 in the continuum limit and obtain

$$J = -\frac{\gamma}{N-1}\sum_{j=1}^{N} z_j I_j(N,\gamma), \quad (41)$$

where

$$I_j(N,\gamma) = \frac{1}{(N+1)^2}\sum_{k_1,k_2=1}^{N}\frac{(1-(-1)^{k_1+k_2})}{\Delta(\beta_1,\beta_2)}\sin(j\beta_1)\sin(j\beta_2)\sin\beta_1\sin\beta_2 \times F\left(\frac{1}{2},\frac{1}{2},1;\,(4\gamma^2/\Delta(\beta_1,\beta_2))^2\right). \quad (42)$$

Using the property that $I_{N+1-j}(N,\gamma) = -I_j(N,\gamma)$ and assuming that N be an even number, eq. (41) simplifies to

$$J = -\frac{\gamma}{N-1}\sum_{j=1}^{N/2}(z_j - z_{N+1-j})\,I_j(N,\gamma). \quad (43)$$

It is known[12] that there is also an energy flow between any intermediate surface and its attached heat bath. Since we are not using the self consistency condition, this intermediate energy fluxes will remain non-zero and affect the per bond average current density J. Consequently, J, as is evident from eq. (43), is dependent on the variables, $\sqrt{\gamma z_2},\cdots,\sqrt{\gamma z_{N-1}}$, the Gaussian widths of the noise functions of the intermediate heat baths. Assume that the widths are such that

$$z_j = z_{N+1-j} \quad \text{for} \quad 2\le j\le N/2. \quad (44)$$

The above conditions imposed on z_js are physically interesting firstly because of the fact that the use of them leads to a heat current density which obeys Fourier's law in the continuum limit. Secondly, the use of them leads to a temperature profile whose nature is similar to what has been observed in Ingen-Hausz's experiment. Thirdly, these conditions, unlike the self consistency conditions used in Ref. 12, allow the radiation to take place in the steady state limit of the transport process. Now the use of these conditions in eq. (36) gives the following relations:

$$z_1 - z_N = \frac{1}{2}\left(\frac{T_1-T_N}{C_{1,1}-C_{N,1}}\right), \quad (45)$$

$$T_j - T_{N+1-j} = \frac{C_{j,1}-C_{N+1-j,1}}{C_{1,1}-C_{N,1}}(T_1-T_N) \quad (46)$$

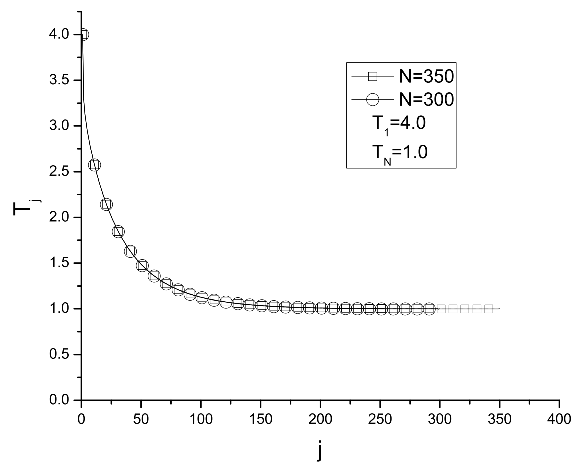

Fig. 1. Temperature profile of the slab for $\gamma = 0.01$.

for $1 \leq j \leq N/2$. Moreover, the use of eq. (44) in (36) reduces N equations into following $N/2$ simultaneous equations of the independent variables z_j ($j = 1, \cdots, N/2$):

$$\sum_{k=1}^{N/2} \bar{C}_{j,k} z_k = \frac{1}{2}\left(T_j + \frac{C_{j,N}}{C_{1,1} - C_{N,1}}(T_1 - T_N)\right), \tag{47}$$

where $j = 1, \cdots, N/2$ and

$$\bar{C}_{j,k} = C_{j,k} + C_{j,N+1-k}. \tag{48}$$

To solve eq. (47) for z_j ($1 \leq j \leq N/2$), we require to know the temperature profile of the slab. The temperatures of the boundary surfaces T_1 and T_N are known and apart from these two, the relations given by eq. (46) provide information about the temperatures of the intermediate surfaces. The profile which is consistent with those relations must be $T_j = T_0 + C_{j,1}(T_1 - T_N)/(C_{1,1} - C_{N,1})$, where T_0 is a constant independent of j. T_0 will be such that T_j equals to T_1 and T_N for j equals to 1 and N respectively. So it gives the temperature profile as

$$T_j = \left[1 - \frac{C_{1,1} + C_{N,1}}{C_{1,1} - C_{N,1}} \frac{T_1 - T_N}{T_1 + T_N}\right] \frac{T_1 + T_N}{2} + \frac{C_{j,1}}{C_{1,1} - C_{N,1}}(T_1 - T_N), \tag{49}$$

where $1 \leq j \leq N$. Moreover, the profile is in conformity with the zeroth law of thermodynamics which tells that $T_j = T_1$ for all j when $T_1 = T_N$. The temperature profile is plotted in Figure (1). Since the profiles become size independent for $N > 300$, the open squares remain coincident with the open circles till $j = 300$. We use eq. (49) in (47) to solve z_j for $j = 1, \cdots, N/2$ and plugging these solutions into

eq. (44) and (45) the rest of z_j for j lying in the range $N/2+1 \leq j \leq N$ are obtained. The result of our numerical evaluations are given in the following table. The Table 1 indicates that z_j are positive definite and size independent for $N \geq 300$.

Table 1. z_j $(1 \leq j \leq N)$ for different N and for $\gamma = 0.01$.

N	z_1	z_j for $2 \leq j \leq N$
300	153.61	1.99
350	153.45	2.0

We use the conditions of eq. (44) into (43) and then using eq. (45) obtain

$$J = -\frac{\gamma}{2(N-1)}\left(\frac{T_1 - T_N}{C_{1,1} - C_{N,1}}\right) I_1(N,\gamma). \tag{50}$$

$I_1(N,\gamma)$ is zero if k_1 and k_2 simultaneously take even integer values or odd integer values. Assuming that N be an even number and using the fact that the summoned of eq. (42) is symmetric in respect of the interchange of β_1 and β_2, we rewrite the double sum of $I_1(N,\gamma)$ as

$$I_1(N,\gamma) = \frac{4}{(N+1)^2}\sum_{j_1,j_2=1}^{N/2}\frac{\sin^2\tilde{\beta}_1\sin^2\tilde{\beta}_2}{\Delta(\tilde{\beta}_1,\tilde{\beta}_2)}F\left(\frac{1}{2},\frac{1}{2},1;\,(4\gamma^2/\Delta(\tilde{\beta}_1,\tilde{\beta}_2))^2\right), \tag{51}$$

where $\tilde{\beta}_1 = 2\pi j_1/(N+1)$ and $\tilde{\beta}_2 = \pi(2j_2-1)/(N+1)$. Again in the continuum limit we convert this double sum into integrals. Defining the integration variables in this limit as $\theta_{1,2} = 2\pi j_{1,2}/(N+1)$, we convert the discrete sums into integrals:

$$\frac{2}{N+1}\sum_{j_{1,2}=1}^{N/2} \to \frac{1}{\pi}\int_0^{\pi} d\theta_{1,2}. \tag{52}$$

$I_1(N,\gamma)$ thus takes the form

$$\begin{aligned} g_1(\gamma) &= \lim_{N\to\infty} I_1(N,\gamma) \\ &= \frac{1}{\pi^2}\int_0^{\pi} d\theta_1 \int_0^{\pi} d\theta_2 \frac{\sin^2\theta_1\sin^2\theta_2}{\Delta(\theta_1,\theta_2)}F\left(\frac{1}{2},\frac{1}{2},1;\,(4\gamma^2/\Delta(\theta_1,\theta_2))^2\right). \end{aligned} \tag{53}$$

Proceeding in the similar manner we obtain the following form of $C_{1,1} - C_{N,1}$ in the continuum limit as

$$\begin{aligned} g_2(\gamma) &= \lim_{N\to\infty}(C_{1,1} - C_{N,1}) \\ &= \frac{1}{\pi^2}\int_0^{\pi} d\theta_1 \int_0^{\pi} d\theta_2 \sin^2\theta_1 \sin^2\theta_2 \frac{\Lambda(\theta_1,\theta_2)}{\Delta(\theta_1,\theta_2)}. \end{aligned} \tag{54}$$

The steady state current density per bond thus reads in the continuum limit as

$$J = -\kappa\frac{(T_1 - T_N)}{N-1}, \tag{55}$$

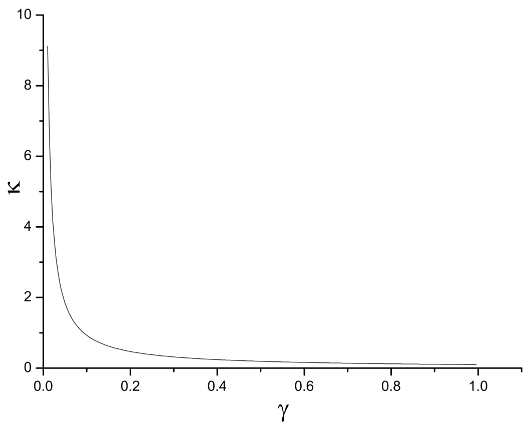

Fig. 2. Plot of κ as a function of γ.

where the conductivity

$$\kappa = \frac{\gamma}{2} \frac{g_1(\gamma)}{g_2(\gamma)}. \tag{56}$$

Here κ is found to be finite and independent of the size of the system. So, as a consequence of the conditions given by eq. (44), Fourier's law holds in the continuum limit. The thermal conductivity κ, as given by eq. (56), is plotted as a function of γ in Figure 2. Here γ appears as a constant in the dissipative force term of the Langevin's equation. Physically it denotes a viscous force experienced by the particles of Brownian like of the slab of crystal owing to collisions with the particles of fluid which seems to constitute the heat baths[15,16]. Moreover, owing to collisions, particles of the slab will experience random forces or noises. Noise does a significant portion of its work in overcoming the viscous drag experienced by a particle of the slab and the rest will be flown as heat energy to the neighbouring particles. Therefore, the increase of γ reduces the rate of flow of heat from a particle to its neighbours and thereby reducing the thermal conductivity of the system. Hence, it justifies reasonably the nature of variation of κ with γ as shown in fig. 2.

According to eq. (49) T_j depends linearly on $C_{j,1}$. We fit $C_{j,1}$ with the following exponentially falling function such a way that

$$C_{j,1} = a_0 + a_1 \mathrm{e}^{-b\,|j-1|}, \tag{57}$$

where a_0, a_1 and b are supposedly N dependent parameters. This parametrized form satisfies all the properties of $C_{j,k}$ given by eq. (35). The numerical values of the parameters for different N are given in the following table. The substitution of eq. (57) into eq. (49) gives the temperature profile of the slab in the thermodynamic

Table 2. Fitting parameters involved with $C_{j,1}$ for different N and for $\gamma = 0.01$.

N	a_0	a_1	b
500	1.48×10^{-5}	4.9868×10^{-3}	0.03220
600	1.48×10^{-5}	4.9872×10^{-3}	0.03212
1000	7.99×10^{-6}	4.9881×10^{-3}	0.03193
2000	3.71×10^{-6}	4.9887×10^{-3}	0.03181
3000	2.41×10^{-6}	4.9889×10^{-3}	0.03177

limit as

$$T_j = T_N + (T_1 - T_N)\mathrm{e}^{-b|j-1|}. \tag{58}$$

It is clear that b is the only parameter which appears in the temperature profile of the slab in the thermodynamic limit and the Table 2 indicates that it approaches to a constant value in this limit. The expression for the profile given by eq. (58) is similar to what has been obtained in the Ingen-Hausz's experiment[14]. Now it is possible to figure out from the temperature profile of the slab the probable physical processes that may take place when heat transports through it. According to Refs. 14, the transport of heat in the steady state limit involves the processes of conduction and radiation of heat. The situation, when the radiation is absent, the temperature falls linearly from left to right boundary surface. On the other hand, if the radiation is allowed to take place, temperature falls exponentially and this very nature is observed in the Ingen-Hausz's experiment. Thus in this paper, allowing the energy fluxes to be flown between the intermediate surfaces and the corresponding heat baths and the use of the conditions given by eq. (44), we are basically allowing the radiation to take place along with the conduction of heat in the steady state limit. If these energy fluxes are not allowed to be flown then a linear variation of temperature is obtained[12]. It implies that the self consistency conditions do not allow the radiation to take place during the steady state transport of heat in the slab.

5. Discussion and conclusion

According to this model, the additional heat baths coupled at the intermediate surfaces and the two baths attached at the boundaries, constitute the surroundings of the slab geometry. The additional heat baths are essentially required to fix the initial state of the slab. When $t >> 1/\gamma$, the slab will attain a unique steady state which is a unison of N different, thermally equilibriated sub-systems, characterized by the temperatures $T_1, \cdots, T_N$. Instead of using self consistent reservoirs[12], we allow the heat fluxes flown between the intermediate surfaces and the corresponding attached heat baths and impose the conditions that the widths of the Gaussian noises of j-th and $N+1-j$-th baths are same for $j = 1, \cdots, N/2$, where N being assumed to be even. Those conditions lead to interesting physically admissible consequences. We show using them that Fourier's law is satisfied in the continuum

limit. Moreover, using those conditions we also obtain a temperature profile, which unlike showing a linear variation of Refs. 12 falls exponentially from left to right end of the slab and this very nature of the profile is also in conformity with that of Ingen-Hausz's experiment. Hence, according to Refs. 14, our model allows the conduction and radiation processes to take place during the steady state transport of heat in the slab.

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